



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:29 AM GMT

PDB ID : 3ES8  
Title : Crystal structure of divergent enolase from *Oceanobacillus Iheyensis* complexed with Mg and L-malate.  
Authors : Fedorov, A.A.; Fedorov, E.V.; Sauder, J.M.; Burley, S.K.; Gerlt, J.A.; Almo, S.C; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-10-04  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

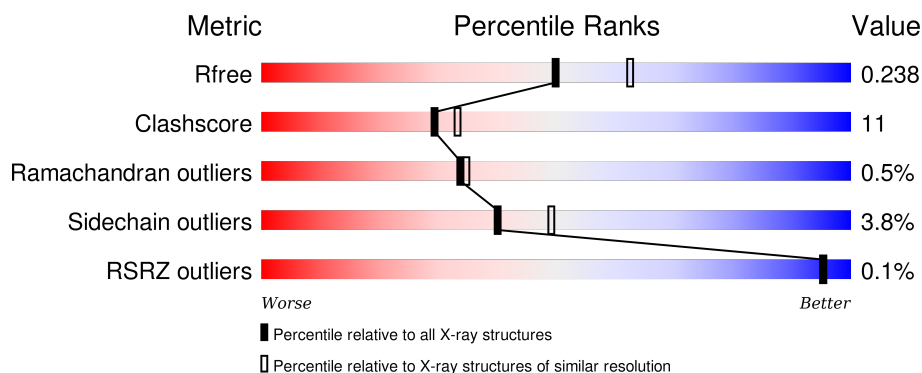
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	391	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	B	391	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	C	391	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	D	391	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	E	391	<div> <div>74%</div> <div>23%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	391	 75%23%..
1	G	391	 75%23%..
1	H	391	 75%23%..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMR	G	392	-	-	-	X
3	MG	F	393	-	-	-	X
3	MG	H	393	-	-	-	X

## 2 Entry composition

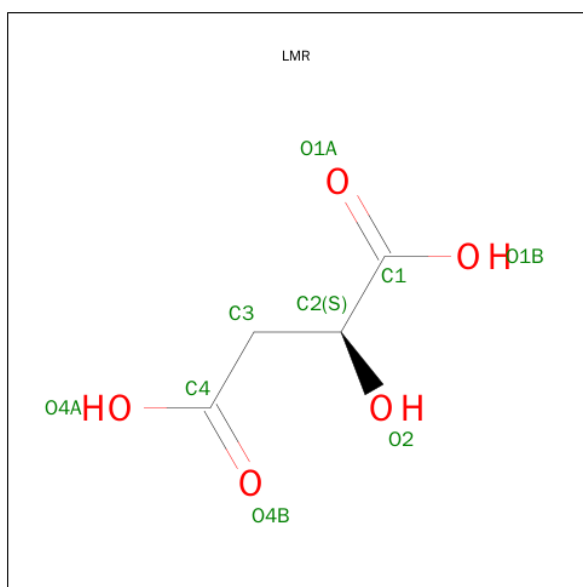
There are 4 unique types of molecules in this entry. The entry contains 25362 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Muconate cycloisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3097	1976	525	586	10			
1	B	387	Total	C	N	O	S	0	0	0
			3097	1976	525	586	10			
1	C	387	Total	C	N	O	S	0	0	0
			3097	1976	525	586	10			
1	D	387	Total	C	N	O	S	0	0	0
			3097	1976	525	586	10			
1	E	387	Total	C	N	O	S	0	0	0
			3097	1976	525	586	10			
1	F	387	Total	C	N	O	S	0	0	0
			3097	1976	525	586	10			
1	G	387	Total	C	N	O	S	0	0	0
			3097	1976	525	586	10			
1	H	387	Total	C	N	O	S	0	0	0
			3097	1976	525	586	10			

- Molecule 2 is (2S)-2-HYDROXYBUTANEDIOIC ACID (three-letter code: LMR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		
2	E	1	Total	C	O	0	0
			9	4	5		
2	F	1	Total	C	O	0	0
			9	4	5		
2	G	1	Total	C	O	0	0
			9	4	5		
2	H	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

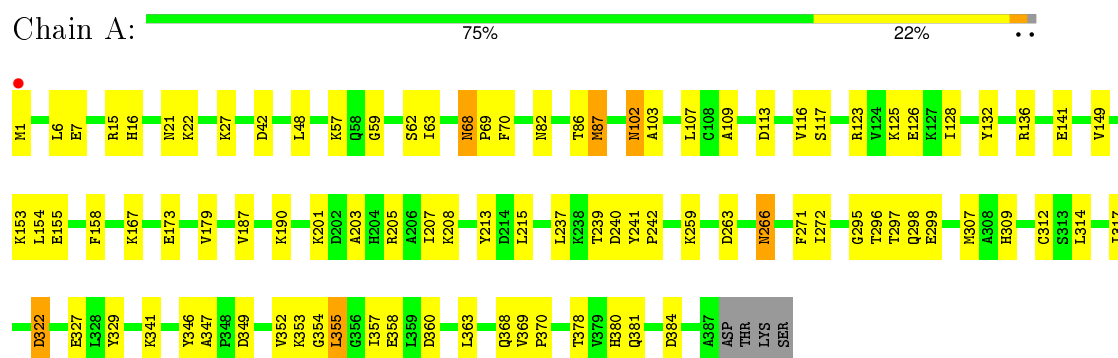
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total 79	O 79	0	0
4	B	50	Total 50	O 50	0	0
4	C	51	Total 51	O 51	0	0
4	D	64	Total 64	O 64	0	0
4	E	69	Total 69	O 69	0	0
4	F	74	Total 74	O 74	0	0
4	G	65	Total 65	O 65	0	0
4	H	54	Total 54	O 54	0	0

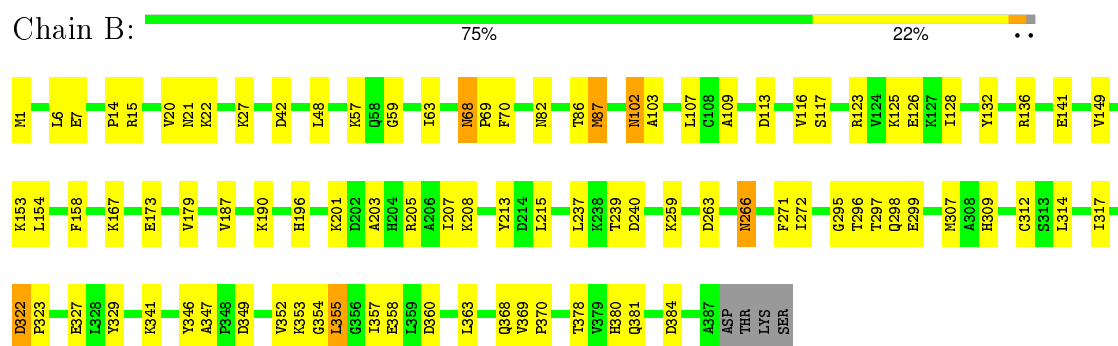
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

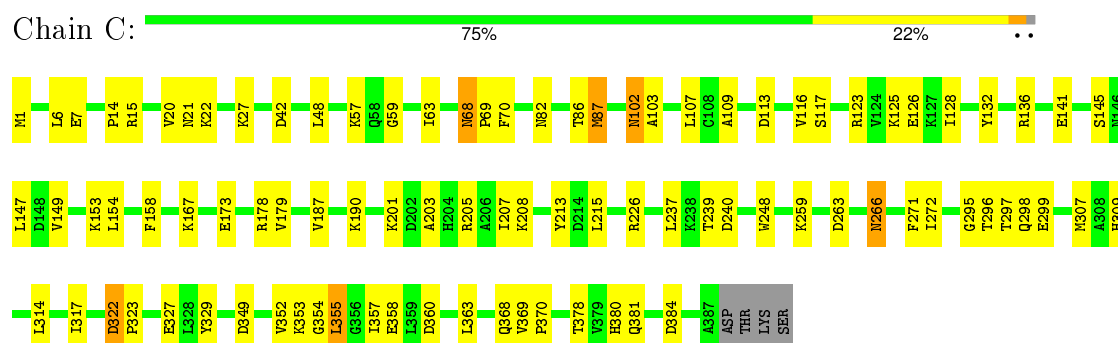
#### • Molecule 1: Muconate cycloisomerase



#### • Molecule 1: Muconate cycloisomerase



#### • Molecule 1: Muconate cycloisomerase



Chain D:

M1	L6	P14	V20	K27	G38	D42	L48	K56	G59	S62	M68	P69	F70	N82	T86	M87	M102	A103	L107	G108	A109	D113	V116	S117	K125	I128	Y132	R136	E141	V149					
K153	L154	F158	K167	E173	V179	V187	K190	K201	T202	A203	K204	K205	A216	L217	K219	D240	K259	D263	D266	F271	I272	G285	T296	T297	Q298	E299	M307	A308	H309	G312	S313	L314	I317	D322	P323
P326	E327	L328	Y329	V338	K341	Y346	A347	P348	D349	V352	K353	G354	L355	G356	I357	E358	L359	D360	L363	Q368	V369	P370	T378	V379	H380	Q381	D384	A387	ASP	THR	LYS	SER			

[illegible][illegible]

Chain G:

75% 23%

M1 L6 E7 P14 R15 H16 V20 I21 K22 K27 D42 L48 K57 Q58 G59 I63 M68 P69 F70 N82 T86 M87 M102 A103 L107 C108 A109 D113 V116 S117 R123 R124 A125 E126 R127 I128 Y132 R136 E141 V140

V150 R151 Q152 K153 L154 F158 K167 E173 V179 E182 V187 K190 K201 D202 A203 E204 R205 A206 I207 K208 Y213 D214 L215 L237 K238 T239 D240 K259 D263 Y266 F271 I272 G295 T296 T297 Q298 E299 K307 A308 H309 L314 L317



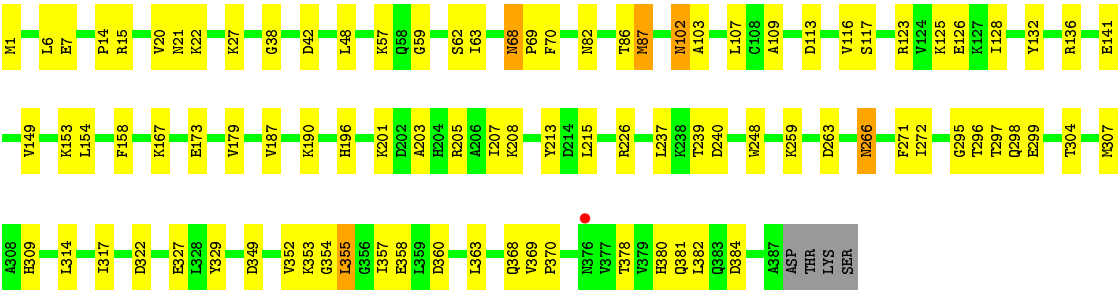
● Molecule 1: Muconate cycloisomerase

Chain H: 

75%

23%

..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.58Å 105.69Å 105.72Å 109.31° 109.47° 109.66°	Depositor
Resolution (Å)	24.94 – 2.20 38.59 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.7 (24.94-2.20) 78.5 (38.59-2.19)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.241 0.221 , 0.238	Depositor DCC
$R_{free}$ test set	8568 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 24.0	EDS
Estimated twinning fraction	0.440 for -k,h+k+l,-h 0.440 for -l,-h,h+k+l 0.002 for -l,h+k+l,-k 0.002 for h+k+l,-l,-h 0.002 for -k,-l,h+k+l 0.002 for h+k+l,-h,-k 0.000 for h,l,-h-k-l 0.000 for h,-h-k-l,k 0.001 for l,h,k 0.001 for k,l,h 0.001 for -h-k-l,k,h 0.001 for l,k,-h-k-l 0.000 for -h-k-l,h,l 0.000 for k,-h-k-l,l 0.470 for -h-k-l,l,k 0.023 for h+k+l,-k,-l 0.024 for k,h,-h-k-l 0.003 for -k,-h,-l 0.024 for l,-h-k-l,h 0.003 for -h,h+k+l,-l 0.022 for -h,-l,-k 0.002 for -h,-k,h+k+l 0.002 for -l,-k,-h	Xtriage

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<sup>1</sup>Intensities estimated from amplitudes.

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Property	Value	Source
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 171840 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	25362	wwPDB-VP
Average B, all atoms ( $\text{\AA}^2$ )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LMR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.37	0/3163	0.64	0/4276
1	B	0.36	0/3163	0.63	0/4276
1	C	0.37	0/3163	0.63	0/4276
1	D	0.36	0/3163	0.64	0/4276
1	E	0.37	0/3163	0.64	0/4276
1	F	0.37	0/3163	0.64	0/4276
1	G	0.36	0/3163	0.63	0/4276
1	H	0.36	0/3163	0.63	0/4276
All	All	0.37	0/25304	0.63	0/34208

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3097	0	3076	78	0
1	B	3097	0	3076	72	0
1	C	3097	0	3076	76	0
1	D	3097	0	3076	73	0
1	E	3097	0	3076	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3097	0	3076	74	0
1	G	3097	0	3076	73	0
1	H	3097	0	3076	75	0
2	A	9	0	3	0	0
2	B	9	0	4	1	0
2	C	9	0	4	1	0
2	D	9	0	3	0	0
2	E	9	0	3	1	0
2	F	9	0	3	0	0
2	G	9	0	3	0	0
2	H	9	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	79	0	0	3	0
4	B	50	0	0	1	0
4	C	51	0	0	1	0
4	D	64	0	0	0	0
4	E	69	0	0	3	0
4	F	74	0	0	1	0
4	G	65	0	0	1	0
4	H	54	0	0	1	0
All	All	25362	0	24634	559	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (559) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ASN:HD21	1:E:295:GLY:HA3	1.17	1.10
1:G:266:ASN:HD21	1:G:295:GLY:HA3	1.17	1.09
1:D:266:ASN:HD21	1:D:295:GLY:HA3	1.17	1.08
1:C:266:ASN:HD21	1:C:295:GLY:HA3	1.16	1.05
1:B:266:ASN:HD21	1:B:295:GLY:HA3	1.16	1.04
1:H:266:ASN:HD21	1:H:295:GLY:HA3	1.17	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:ASN:HD21	1:F:295:GLY:HA3	1.18	1.02
1:A:266:ASN:HD21	1:A:295:GLY:HA3	1.19	1.01
1:A:102:ASN:HD22	1:A:103:ALA:N	1.75	0.85
1:E:102:ASN:HD22	1:E:103:ALA:N	1.74	0.85
1:C:102:ASN:HD22	1:C:103:ALA:N	1.74	0.84
1:D:102:ASN:HD22	1:D:103:ALA:N	1.74	0.84
1:B:102:ASN:HD22	1:B:103:ALA:N	1.74	0.84
1:G:102:ASN:HD22	1:G:103:ALA:N	1.75	0.83
1:F:102:ASN:HD22	1:F:103:ALA:N	1.76	0.83
1:H:102:ASN:HD22	1:H:103:ALA:N	1.75	0.83
1:A:155:GLU:HG3	4:A:398:HOH:O	1.85	0.77
1:C:266:ASN:HD21	1:C:295:GLY:CA	1.99	0.76
1:H:266:ASN:HD21	1:H:295:GLY:CA	2.00	0.74
1:B:266:ASN:HD21	1:B:295:GLY:CA	1.99	0.74
1:D:266:ASN:HD21	1:D:295:GLY:CA	2.00	0.72
1:D:266:ASN:HD22	1:D:266:ASN:C	1.95	0.70
1:D:117:SER:OG	1:D:309:HIS:HD2	1.75	0.70
1:A:173:GLU:HG3	1:A:213:TYR:HE2	1.57	0.69
1:F:266:ASN:C	1:F:266:ASN:HD22	1.96	0.69
1:G:173:GLU:HG3	1:G:213:TYR:HE2	1.58	0.69
1:B:266:ASN:ND2	1:B:295:GLY:HA3	2.01	0.69
1:F:22:LYS:HE2	1:F:369:VAL:HG11	1.75	0.69
1:B:266:ASN:C	1:B:266:ASN:HD22	1.96	0.69
1:A:266:ASN:HD22	1:A:266:ASN:C	1.95	0.69
1:C:266:ASN:C	1:C:266:ASN:HD22	1.97	0.68
1:F:173:GLU:HG3	1:F:213:TYR:HE2	1.57	0.68
1:E:15:ARG:NE	1:E:21:ASN:HD21	1.91	0.68
1:G:22:LYS:HE2	1:G:369:VAL:HG11	1.76	0.68
1:H:173:GLU:HG3	1:H:213:TYR:HE2	1.59	0.68
1:G:266:ASN:HD21	1:G:295:GLY:CA	2.00	0.68
1:E:196:HIS:HD2	4:E:445:HOH:O	1.77	0.68
1:F:266:ASN:HD21	1:F:295:GLY:CA	2.01	0.68
1:B:196:HIS:HD2	4:B:423:HOH:O	1.76	0.68
1:A:167:LYS:NZ	1:A:380:HIS:HD2	1.92	0.67
1:F:314:LEU:HD12	1:F:317:ILE:HD11	1.76	0.67
1:B:173:GLU:HG3	1:B:213:TYR:HE2	1.59	0.67
1:C:314:LEU:HD12	1:C:317:ILE:HD11	1.76	0.67
1:E:173:GLU:HG3	1:E:213:TYR:HE2	1.59	0.67
1:D:22:LYS:HE2	1:D:369:VAL:HG11	1.76	0.67
1:H:266:ASN:C	1:H:266:ASN:HD22	1.97	0.67
1:A:314:LEU:HD12	1:A:317:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ASN:HD22	1:E:266:ASN:C	1.98	0.67
1:H:15:ARG:NE	1:H:21:ASN:HD21	1.92	0.67
1:C:173:GLU:HG3	1:C:213:TYR:HE2	1.60	0.67
1:B:15:ARG:NE	1:B:21:ASN:HD21	1.92	0.67
1:E:266:ASN:HD21	1:E:295:GLY:CA	2.01	0.67
1:C:117:SER:OG	1:C:309:HIS:HD2	1.77	0.67
1:G:117:SER:OG	1:G:309:HIS:HD2	1.78	0.67
1:D:314:LEU:HD12	1:D:317:ILE:HD11	1.76	0.66
1:G:266:ASN:HD22	1:G:266:ASN:C	1.98	0.66
1:E:167:LYS:NZ	1:E:380:HIS:HD2	1.93	0.66
1:A:117:SER:OG	1:A:309:HIS:HD2	1.77	0.66
1:B:117:SER:OG	1:B:309:HIS:HD2	1.78	0.66
1:E:314:LEU:HD12	1:E:317:ILE:HD11	1.78	0.66
1:D:266:ASN:ND2	1:D:295:GLY:HA3	2.01	0.66
1:E:117:SER:OG	1:E:309:HIS:HD2	1.78	0.66
1:F:117:SER:OG	1:F:309:HIS:HD2	1.77	0.66
1:H:167:LYS:NZ	1:H:380:HIS:HD2	1.94	0.66
1:F:167:LYS:NZ	1:F:380:HIS:HD2	1.93	0.66
1:B:314:LEU:HD12	1:B:317:ILE:HD11	1.77	0.66
1:H:117:SER:OG	1:H:309:HIS:HD2	1.78	0.65
1:D:173:GLU:HG3	1:D:213:TYR:HE2	1.59	0.65
1:C:15:ARG:NE	1:C:21:ASN:HD21	1.94	0.65
1:C:167:LYS:NZ	1:C:380:HIS:HD2	1.95	0.65
1:A:22:LYS:HE2	1:A:369:VAL:HG11	1.78	0.65
1:G:167:LYS:NZ	1:G:380:HIS:HD2	1.95	0.65
1:A:15:ARG:NE	1:A:21:ASN:HD21	1.95	0.65
1:G:314:LEU:HD12	1:G:317:ILE:HD11	1.77	0.65
1:B:22:LYS:HE2	1:B:369:VAL:HG11	1.78	0.65
1:G:15:ARG:NE	1:G:21:ASN:HD21	1.95	0.65
1:H:314:LEU:HD12	1:H:317:ILE:HD11	1.77	0.64
1:C:266:ASN:ND2	1:C:295:GLY:HA3	2.01	0.64
1:B:167:LYS:NZ	1:B:380:HIS:HD2	1.95	0.64
1:F:266:ASN:ND2	1:F:295:GLY:HA3	2.03	0.64
1:F:15:ARG:NE	1:F:21:ASN:HD21	1.95	0.64
1:A:266:ASN:ND2	1:A:295:GLY:HA3	2.03	0.63
1:C:22:LYS:HE2	1:C:369:VAL:HG11	1.81	0.63
1:H:196:HIS:HD2	4:H:447:HOH:O	1.81	0.62
1:D:167:LYS:NZ	1:D:380:HIS:HD2	1.97	0.62
1:A:266:ASN:HD21	1:A:295:GLY:CA	2.03	0.62
1:D:15:ARG:NE	1:D:21:ASN:HD21	1.97	0.62
1:H:22:LYS:HE2	1:H:369:VAL:HG11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ASN:ND2	1:E:295:GLY:HA3	2.01	0.62
1:E:22:LYS:HE2	1:E:369:VAL:HG11	1.82	0.61
1:G:102:ASN:HD22	1:G:103:ALA:H	1.47	0.61
1:F:102:ASN:HD22	1:F:103:ALA:H	1.48	0.61
1:A:102:ASN:HD22	1:A:103:ALA:H	1.47	0.60
1:G:266:ASN:ND2	1:G:295:GLY:HA3	2.02	0.60
1:A:240:ASP:OD1	1:G:208:LYS:HE3	2.01	0.60
1:B:86:THR:O	1:G:86:THR:O	2.19	0.60
1:B:378:THR:OG1	1:B:381:GLN:HG3	2.02	0.60
1:C:102:ASN:HD22	1:C:103:ALA:H	1.50	0.60
1:D:208:LYS:HE3	1:F:240:ASP:OD1	2.02	0.60
1:D:86:THR:O	1:E:86:THR:O	2.19	0.60
1:H:266:ASN:ND2	1:H:295:GLY:HA3	2.02	0.60
1:E:378:THR:OG1	1:E:381:GLN:HG3	2.02	0.60
1:H:378:THR:OG1	1:H:381:GLN:HG3	2.02	0.60
1:D:102:ASN:HD22	1:D:103:ALA:H	1.48	0.59
1:E:15:ARG:HE	1:E:21:ASN:ND2	2.00	0.59
1:G:378:THR:OG1	1:G:381:GLN:HG3	2.03	0.59
1:E:102:ASN:HD22	1:E:103:ALA:H	1.47	0.59
1:A:173:GLU:HG3	1:A:213:TYR:CE2	2.37	0.59
1:G:173:GLU:HG3	1:G:213:TYR:CE2	2.37	0.59
1:E:188:ARG:HD2	4:E:424:HOH:O	2.02	0.59
1:H:102:ASN:HD22	1:H:103:ALA:H	1.50	0.58
1:H:15:ARG:HE	1:H:21:ASN:ND2	2.02	0.58
1:A:86:THR:O	1:C:86:THR:O	2.21	0.58
1:H:173:GLU:HG3	1:H:213:TYR:CE2	2.39	0.58
1:D:378:THR:OG1	1:D:381:GLN:HG3	2.02	0.58
1:F:173:GLU:HG3	1:F:213:TYR:CE2	2.37	0.58
1:A:378:THR:OG1	1:A:381:GLN:HG3	2.03	0.58
1:C:378:THR:OG1	1:C:381:GLN:HG3	2.04	0.58
1:F:86:THR:O	1:H:86:THR:O	2.21	0.58
1:B:102:ASN:HD22	1:B:103:ALA:H	1.49	0.58
1:C:173:GLU:HG3	1:C:213:TYR:CE2	2.39	0.58
1:E:173:GLU:HG3	1:E:213:TYR:CE2	2.39	0.57
1:F:378:THR:OG1	1:F:381:GLN:HG3	2.04	0.57
1:A:68:ASN:HD22	1:A:68:ASN:C	2.08	0.57
1:F:201:LYS:HD3	1:G:263:ASP:OD2	2.05	0.57
1:D:201:LYS:HD3	1:F:263:ASP:OD2	2.04	0.57
1:C:68:ASN:HD22	1:C:69:PRO:CD	2.18	0.57
1:A:136:ARG:HD2	1:A:384:ASP:OD1	2.05	0.57
1:A:309:HIS:HE1	1:A:355:LEU:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:VAL:HG13	1:E:370:PRO:HD2	1.87	0.56
1:D:68:ASN:HD22	1:D:69:PRO:CD	2.19	0.56
1:D:215:LEU:N	1:D:215:LEU:HD12	2.21	0.56
1:F:68:ASN:HD22	1:F:69:PRO:CD	2.18	0.56
1:B:15:ARG:HE	1:B:21:ASN:ND2	2.02	0.56
1:A:215:LEU:HD12	1:A:215:LEU:N	2.21	0.56
1:B:136:ARG:HD2	1:B:384:ASP:OD1	2.05	0.56
1:F:208:LYS:HE3	1:G:240:ASP:OD1	2.04	0.56
1:D:173:GLU:HG3	1:D:213:TYR:CE2	2.39	0.56
1:B:173:GLU:HG3	1:B:213:TYR:CE2	2.38	0.56
1:G:309:HIS:HE1	1:G:355:LEU:O	1.88	0.56
1:C:136:ARG:HD2	1:C:384:ASP:OD1	2.05	0.56
1:G:15:ARG:HE	1:G:21:ASN:ND2	2.04	0.56
1:G:68:ASN:C	1:G:68:ASN:HD22	2.10	0.56
1:A:208:LYS:HE3	1:D:240:ASP:OD1	2.06	0.56
1:A:15:ARG:HE	1:A:21:ASN:ND2	2.04	0.56
1:F:87:MET:HB3	1:H:87:MET:HB3	1.88	0.56
1:F:68:ASN:C	1:F:68:ASN:HD22	2.08	0.55
1:H:136:ARG:HD2	1:H:384:ASP:OD1	2.05	0.55
1:E:68:ASN:HD22	1:E:69:PRO:CD	2.19	0.55
1:G:215:LEU:N	1:G:215:LEU:HD12	2.21	0.55
1:F:215:LEU:HD12	1:F:215:LEU:N	2.21	0.55
1:F:309:HIS:HE1	1:F:355:LEU:O	1.89	0.55
1:F:15:ARG:HE	1:F:21:ASN:ND2	2.04	0.55
1:A:68:ASN:HD22	1:A:69:PRO:CD	2.19	0.55
1:D:309:HIS:HE1	1:D:355:LEU:O	1.89	0.55
1:H:68:ASN:HD22	1:H:69:PRO:CD	2.19	0.55
1:H:68:ASN:C	1:H:68:ASN:HD22	2.10	0.55
1:H:309:HIS:HE1	1:H:355:LEU:O	1.89	0.55
1:F:136:ARG:HD2	1:F:384:ASP:OD1	2.07	0.55
1:C:68:ASN:C	1:C:68:ASN:HD22	2.10	0.55
1:B:68:ASN:C	1:B:68:ASN:HD22	2.10	0.55
1:B:68:ASN:HD22	1:B:69:PRO:CD	2.19	0.55
1:B:296:THR:HG22	1:B:322:ASP:HB2	1.88	0.55
1:E:309:HIS:HE1	1:E:355:LEU:O	1.90	0.54
1:B:15:ARG:HE	1:B:21:ASN:HD21	1.55	0.54
1:C:15:ARG:HE	1:C:21:ASN:ND2	2.05	0.54
1:A:87:MET:HB3	1:C:87:MET:HB3	1.89	0.54
1:A:263:ASP:OD2	1:G:201:LYS:HD3	2.07	0.54
1:F:205:ARG:HD3	1:G:240:ASP:O	2.07	0.54
1:E:136:ARG:HD2	1:E:384:ASP:OD1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LYS:HD3	1:D:263:ASP:OD2	2.07	0.54
1:G:296:THR:HG22	1:G:322:ASP:HB2	1.90	0.54
1:C:68:ASN:HD22	1:C:69:PRO:HD2	1.72	0.54
1:C:309:HIS:HE1	1:C:355:LEU:O	1.91	0.54
1:F:369:VAL:HG13	1:F:370:PRO:HD2	1.90	0.54
1:H:369:VAL:HG13	1:H:370:PRO:HD2	1.89	0.54
1:A:369:VAL:HG13	1:A:370:PRO:HD2	1.88	0.54
1:D:87:MET:HB3	1:E:87:MET:HB3	1.89	0.54
1:D:68:ASN:C	1:D:68:ASN:HD22	2.10	0.54
1:G:369:VAL:HG13	1:G:370:PRO:HD2	1.90	0.53
1:B:309:HIS:HE1	1:B:355:LEU:O	1.91	0.53
1:D:68:ASN:HD22	1:D:69:PRO:HD2	1.72	0.53
1:A:296:THR:HG22	1:A:322:ASP:HB2	1.91	0.53
1:E:15:ARG:HE	1:E:21:ASN:HD21	1.53	0.53
1:B:68:ASN:HD22	1:B:69:PRO:HD2	1.73	0.53
1:H:215:LEU:N	1:H:215:LEU:HD12	2.24	0.53
1:F:132:TYR:CE2	1:F:153:LYS:HE2	2.43	0.53
1:B:87:MET:HB3	1:G:87:MET:HB3	1.89	0.53
1:G:136:ARG:HD2	1:G:384:ASP:OD1	2.08	0.53
1:B:215:LEU:HD12	1:B:215:LEU:N	2.23	0.53
1:H:68:ASN:HD22	1:H:69:PRO:HD2	1.73	0.53
1:A:349:ASP:HB3	1:A:352:VAL:HG23	1.91	0.53
1:H:349:ASP:HB3	1:H:352:VAL:HG23	1.91	0.53
1:D:132:TYR:CE2	1:D:153:LYS:HE2	2.43	0.53
1:C:215:LEU:N	1:C:215:LEU:HD12	2.23	0.53
1:D:369:VAL:HG13	1:D:370:PRO:HD2	1.89	0.53
1:C:369:VAL:HG13	1:C:370:PRO:HD2	1.91	0.53
1:F:68:ASN:HD22	1:F:69:PRO:HD2	1.73	0.53
1:G:68:ASN:HD22	1:G:69:PRO:CD	2.21	0.53
1:E:68:ASN:HD22	1:E:68:ASN:C	2.11	0.53
1:C:296:THR:HG22	1:C:322:ASP:HB2	1.91	0.53
1:D:136:ARG:HD2	1:D:384:ASP:OD1	2.09	0.53
1:E:349:ASP:HB3	1:E:352:VAL:HG23	1.91	0.53
1:A:68:ASN:HD22	1:A:69:PRO:HD2	1.74	0.52
1:E:68:ASN:HD22	1:E:69:PRO:HD2	1.73	0.52
1:F:296:THR:HG22	1:F:322:ASP:HB2	1.89	0.52
1:B:349:ASP:HB3	1:B:352:VAL:HG23	1.92	0.52
1:B:369:VAL:HG13	1:B:370:PRO:HD2	1.91	0.52
1:F:15:ARG:HE	1:F:21:ASN:HD21	1.58	0.52
1:D:15:ARG:HE	1:D:21:ASN:ND2	2.08	0.52
1:G:349:ASP:HB3	1:G:352:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:THR:HG22	1:D:322:ASP:HB2	1.91	0.51
1:F:349:ASP:HB3	1:F:352:VAL:HG23	1.92	0.51
1:G:7:GLU:HB2	1:G:27:LYS:HB2	1.92	0.51
1:E:215:LEU:HD12	1:E:215:LEU:N	2.24	0.51
1:H:102:ASN:HD22	1:H:102:ASN:C	2.14	0.51
1:H:15:ARG:HE	1:H:21:ASN:HD21	1.54	0.51
1:G:132:TYR:CE2	1:G:153:LYS:HE2	2.45	0.51
1:C:132:TYR:CE2	1:C:153:LYS:HE2	2.45	0.51
1:G:68:ASN:HD22	1:G:69:PRO:HD2	1.76	0.51
1:A:109:ALA:HB3	1:A:354:GLY:HA2	1.93	0.51
1:A:132:TYR:CE2	1:A:153:LYS:HE2	2.45	0.51
1:H:132:TYR:CE2	1:H:153:LYS:HE2	2.46	0.51
1:H:296:THR:HG22	1:H:322:ASP:HB2	1.92	0.51
1:D:7:GLU:HB2	1:D:27:LYS:HB2	1.92	0.51
1:A:167:LYS:HZ3	1:A:380:HIS:HD2	1.58	0.51
1:A:68:ASN:HD22	1:A:69:PRO:N	2.09	0.51
1:B:132:TYR:CE2	1:B:153:LYS:HE2	2.46	0.51
1:A:158:PHE:HZ	1:A:327:GLU:HG3	1.76	0.51
1:B:240:ASP:OD1	1:C:208:LYS:HE3	2.12	0.50
1:E:109:ALA:HB3	1:E:354:GLY:HA2	1.93	0.50
1:C:7:GLU:HB2	1:C:27:LYS:HB2	1.93	0.50
1:E:296:THR:HG22	1:E:322:ASP:HB2	1.91	0.50
1:F:7:GLU:HB2	1:F:27:LYS:HB2	1.93	0.50
1:B:7:GLU:HB2	1:B:27:LYS:HB2	1.91	0.50
1:C:349:ASP:HB3	1:C:352:VAL:HG23	1.93	0.50
1:E:7:GLU:HB2	1:E:27:LYS:HB2	1.92	0.50
1:A:7:GLU:HB2	1:A:27:LYS:HB2	1.93	0.50
1:D:349:ASP:HB3	1:D:352:VAL:HG23	1.93	0.50
1:A:15:ARG:HE	1:A:21:ASN:HD21	1.59	0.50
1:H:271:PHE:CZ	1:H:297:THR:HB	2.47	0.50
1:F:109:ALA:HB3	1:F:354:GLY:HA2	1.93	0.50
1:E:21:ASN:HD22	1:E:329:TYR:HE1	1.59	0.50
1:C:158:PHE:HZ	1:C:327:GLU:HG3	1.76	0.50
1:E:298:GLN:HA	1:E:298:GLN:OE1	2.11	0.50
1:B:167:LYS:HZ1	1:B:380:HIS:HD2	1.59	0.50
1:E:167:LYS:HZ3	1:E:380:HIS:HD2	1.60	0.50
1:B:109:ALA:HB3	1:B:354:GLY:HA2	1.94	0.49
1:F:158:PHE:HZ	1:F:327:GLU:HG3	1.76	0.49
1:A:205:ARG:HD3	1:D:240:ASP:O	2.11	0.49
1:G:271:PHE:CZ	1:G:297:THR:HB	2.47	0.49
1:F:271:PHE:CZ	1:F:297:THR:HB	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:PHE:HZ	1:E:327:GLU:HG3	1.77	0.49
1:B:102:ASN:C	1:B:102:ASN:HD22	2.13	0.49
1:A:271:PHE:CZ	1:A:297:THR:HB	2.47	0.49
1:C:68:ASN:HD22	1:C:69:PRO:N	2.11	0.49
1:G:109:ALA:HB3	1:G:354:GLY:HA2	1.93	0.49
1:H:7:GLU:HB2	1:H:27:LYS:HB2	1.93	0.49
1:A:167:LYS:HZ3	1:A:380:HIS:CD2	2.30	0.49
1:F:68:ASN:HD22	1:F:69:PRO:N	2.09	0.49
1:H:158:PHE:HZ	1:H:327:GLU:HG3	1.77	0.49
1:E:132:TYR:CE2	1:E:153:LYS:HE2	2.48	0.49
1:G:158:PHE:HZ	1:G:327:GLU:HG3	1.78	0.49
1:H:21:ASN:HD22	1:H:329:TYR:HE1	1.60	0.49
1:E:116:VAL:HG21	1:E:355:LEU:CD1	2.43	0.49
1:H:68:ASN:HD22	1:H:69:PRO:N	2.10	0.49
1:C:271:PHE:CZ	1:C:297:THR:HB	2.48	0.49
1:B:21:ASN:HD22	1:B:329:TYR:HE1	1.60	0.49
1:D:205:ARG:HD3	1:F:240:ASP:O	2.13	0.49
1:G:68:ASN:HD22	1:G:69:PRO:N	2.10	0.48
1:D:158:PHE:HZ	1:D:327:GLU:HG3	1.77	0.48
1:D:179:VAL:CG1	1:D:187:VAL:HG21	2.43	0.48
1:H:109:ALA:HB3	1:H:354:GLY:HA2	1.95	0.48
1:B:158:PHE:HZ	1:B:327:GLU:HG3	1.77	0.48
1:D:68:ASN:HD22	1:D:69:PRO:N	2.10	0.48
1:B:201:LYS:HD3	1:H:263:ASP:OD2	2.13	0.48
1:H:298:GLN:OE1	1:H:298:GLN:HA	2.13	0.48
1:D:271:PHE:CZ	1:D:297:THR:HB	2.49	0.48
1:C:109:ALA:HB3	1:C:354:GLY:HA2	1.94	0.48
1:B:116:VAL:HG21	1:B:355:LEU:CD1	2.42	0.48
1:D:109:ALA:HB3	1:D:354:GLY:HA2	1.94	0.48
1:A:298:GLN:OE1	1:A:298:GLN:HA	2.13	0.48
1:F:16:HIS:HE1	4:F:406:HOH:O	1.95	0.48
1:G:16:HIS:HE1	4:G:426:HOH:O	1.95	0.48
1:E:240:ASP:OD1	1:H:208:LYS:HE3	2.14	0.48
1:C:59:GLY:O	1:C:63:ILE:HG12	2.14	0.48
1:E:68:ASN:HD22	1:E:69:PRO:N	2.11	0.48
1:E:167:LYS:HZ3	1:E:380:HIS:CD2	2.32	0.48
1:B:271:PHE:CZ	1:B:297:THR:HB	2.48	0.48
1:G:179:VAL:CG1	1:G:187:VAL:HG21	2.44	0.47
1:H:116:VAL:HG21	1:H:355:LEU:CD1	2.44	0.47
1:B:208:LYS:HE3	1:H:240:ASP:OD1	2.14	0.47
1:A:299:GLU:OE2	1:A:307:MET:SD	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:ARG:NH1	1:G:182:GLU:OE2	2.39	0.47
1:A:125:LYS:HD2	1:A:128:ILE:HG22	1.97	0.47
1:B:240:ASP:O	1:C:205:ARG:HD3	2.15	0.47
1:B:59:GLY:O	1:B:63:ILE:HG12	2.14	0.47
1:F:59:GLY:O	1:F:63:ILE:HG12	2.15	0.47
1:G:59:GLY:O	1:G:63:ILE:HG12	2.14	0.47
1:B:68:ASN:HD22	1:B:69:PRO:N	2.12	0.47
1:D:59:GLY:O	1:D:63:ILE:HG12	2.15	0.47
1:D:116:VAL:HG21	1:D:355:LEU:CD1	2.45	0.47
1:C:116:VAL:HG21	1:C:355:LEU:CD1	2.45	0.47
1:A:240:ASP:O	1:G:205:ARG:HD3	2.15	0.47
1:E:271:PHE:CZ	1:E:297:THR:HB	2.49	0.47
1:E:357:ILE:CG2	1:E:358:GLU:N	2.78	0.47
1:C:298:GLN:HA	1:C:298:GLN:OE1	2.15	0.47
1:A:179:VAL:CG1	1:A:187:VAL:HG21	2.44	0.47
1:A:59:GLY:O	1:A:63:ILE:HG12	2.15	0.47
1:C:21:ASN:HD22	1:C:329:TYR:HE1	1.63	0.47
1:G:21:ASN:HD22	1:G:329:TYR:HE1	1.62	0.47
1:D:82:ASN:ND2	1:E:48:LEU:HD22	2.30	0.47
1:A:82:ASN:ND2	1:C:48:LEU:HD22	2.29	0.47
1:F:179:VAL:CG1	1:F:187:VAL:HG21	2.45	0.47
1:D:299:GLU:OE2	1:D:307:MET:SD	2.73	0.47
1:C:240:ASP:OD1	1:E:208:LYS:HE3	2.16	0.47
1:D:102:ASN:HD22	1:D:102:ASN:C	2.13	0.46
1:B:263:ASP:OD2	1:C:201:LYS:HD3	2.15	0.46
1:B:298:GLN:OE1	1:B:298:GLN:HA	2.14	0.46
1:G:299:GLU:OE2	1:G:307:MET:SD	2.73	0.46
1:D:149:VAL:O	1:D:153:LYS:HG2	2.16	0.46
1:H:357:ILE:CG2	1:H:358:GLU:N	2.78	0.46
1:B:179:VAL:CG1	1:B:187:VAL:HG21	2.45	0.46
1:C:357:ILE:CG2	1:C:358:GLU:N	2.78	0.46
1:H:179:VAL:CG1	1:H:187:VAL:HG21	2.45	0.46
1:D:266:ASN:ND2	1:D:266:ASN:C	2.67	0.46
1:F:298:GLN:OE1	1:F:298:GLN:HA	2.15	0.46
1:G:298:GLN:OE1	1:G:298:GLN:HA	2.14	0.46
1:E:59:GLY:O	1:E:63:ILE:HG12	2.15	0.46
1:F:299:GLU:OE2	1:F:307:MET:SD	2.73	0.46
1:F:82:ASN:ND2	1:H:48:LEU:HD22	2.31	0.46
1:G:22:LYS:CE	1:G:369:VAL:HG11	2.45	0.46
1:C:179:VAL:HG13	1:C:187:VAL:HG21	1.98	0.46
1:C:179:VAL:CG1	1:C:187:VAL:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ILE:CG2	1:B:358:GLU:N	2.78	0.46
1:H:167:LYS:HZ1	1:H:380:HIS:HD2	1.63	0.46
1:E:263:ASP:OD2	1:H:201:LYS:HD3	2.15	0.46
1:F:102:ASN:HD22	1:F:102:ASN:C	2.17	0.46
1:F:116:VAL:HG21	1:F:355:LEU:CD1	2.45	0.46
1:F:21:ASN:HD22	1:F:329:TYR:HE1	1.64	0.46
1:A:149:VAL:O	1:A:153:LYS:HG2	2.16	0.46
1:A:155:GLU:CG	4:A:398:HOH:O	2.54	0.45
1:E:240:ASP:O	1:H:205:ARG:HD3	2.16	0.45
1:A:179:VAL:HG13	1:A:187:VAL:HG21	1.98	0.45
1:A:102:ASN:HD22	1:A:102:ASN:C	2.15	0.45
1:F:22:LYS:CE	1:F:369:VAL:HG11	2.44	0.45
1:G:116:VAL:HG21	1:G:355:LEU:CD1	2.46	0.45
1:G:149:VAL:O	1:G:153:LYS:HG2	2.16	0.45
1:C:299:GLU:OE2	1:C:307:MET:SD	2.74	0.45
1:A:116:VAL:HG21	1:A:355:LEU:CD1	2.46	0.45
1:C:167:LYS:HZ1	1:C:380:HIS:HD2	1.63	0.45
1:G:360:ASP:HB3	1:G:363:LEU:HD12	1.99	0.45
1:B:48:LEU:HD22	1:G:82:ASN:ND2	2.32	0.45
1:D:360:ASP:HB3	1:D:363:LEU:HD12	1.99	0.45
1:B:299:GLU:OE2	1:B:307:MET:SD	2.75	0.45
1:B:125:LYS:HD2	1:B:128:ILE:HG22	1.98	0.45
1:A:21:ASN:HD22	1:A:329:TYR:HE1	1.65	0.45
1:G:357:ILE:CG2	1:G:358:GLU:N	2.79	0.45
1:A:357:ILE:CG2	1:A:358:GLU:N	2.79	0.45
1:E:113:ASP:OD1	1:E:353:LYS:HE2	2.17	0.45
1:H:113:ASP:OD1	1:H:353:LYS:HE2	2.17	0.45
1:E:21:ASN:ND2	1:E:329:TYR:HE1	2.15	0.45
1:F:167:LYS:HZ1	1:F:380:HIS:HD2	1.62	0.45
1:F:179:VAL:HG13	1:F:187:VAL:HG21	1.99	0.45
1:H:360:ASP:HB3	1:H:363:LEU:HD12	1.99	0.45
1:A:272:ILE:O	1:A:272:ILE:HG13	2.17	0.45
1:E:179:VAL:CG1	1:E:187:VAL:HG21	2.46	0.45
1:G:167:LYS:HZ3	1:G:380:HIS:HD2	1.65	0.45
1:E:179:VAL:HG13	1:E:187:VAL:HG21	1.99	0.45
1:D:272:ILE:HG13	1:D:272:ILE:O	2.17	0.45
1:E:360:ASP:HB3	1:E:363:LEU:HD12	1.98	0.45
1:E:102:ASN:HD22	1:E:102:ASN:C	2.13	0.45
1:D:167:LYS:HZ3	1:D:380:HIS:HD2	1.65	0.45
1:G:125:LYS:HD2	1:G:128:ILE:HG22	1.99	0.45
1:E:299:GLU:OE2	1:E:307:MET:SD	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:GLY:O	1:H:63:ILE:HG12	2.16	0.45
1:F:167:LYS:HZ3	1:F:380:HIS:CD2	2.36	0.44
1:A:68:ASN:ND2	1:A:70:PHE:H	2.14	0.44
1:F:68:ASN:ND2	1:F:70:PHE:H	2.15	0.44
1:B:297:THR:HA	2:B:392:LMR:O2	2.17	0.44
1:C:125:LYS:HD2	1:C:128:ILE:HG22	1.99	0.44
1:E:125:LYS:HD2	1:E:128:ILE:HG22	1.99	0.44
1:C:263:ASP:OD2	1:E:201:LYS:HD3	2.16	0.44
1:E:272:ILE:HG13	1:E:272:ILE:O	2.17	0.44
1:F:357:ILE:CG2	1:F:358:GLU:N	2.81	0.44
1:E:68:ASN:ND2	1:E:70:PHE:H	2.16	0.44
1:H:68:ASN:ND2	1:H:70:PHE:H	2.15	0.44
1:C:360:ASP:HB3	1:C:363:LEU:HD12	1.99	0.44
1:B:179:VAL:HG13	1:B:187:VAL:HG21	1.99	0.44
1:A:360:ASP:HB3	1:A:363:LEU:HD12	1.98	0.44
1:E:167:LYS:HZ1	1:E:380:HIS:HD2	1.65	0.44
1:C:158:PHE:CZ	1:C:327:GLU:HG3	2.51	0.44
1:G:179:VAL:HG13	1:G:187:VAL:HG21	2.00	0.44
1:D:113:ASP:OD1	1:D:353:LYS:HE2	2.17	0.44
1:D:298:GLN:OE1	1:D:298:GLN:HA	2.17	0.44
1:B:21:ASN:ND2	1:B:329:TYR:HE1	2.15	0.44
1:B:158:PHE:CZ	1:B:327:GLU:HG3	2.52	0.44
1:F:312:CYS:SG	1:F:347:ALA:HB2	2.58	0.44
1:A:22:LYS:CE	1:A:369:VAL:HG11	2.45	0.44
1:D:21:ASN:HD22	1:D:329:TYR:HE1	1.64	0.44
1:G:68:ASN:ND2	1:G:70:PHE:H	2.15	0.44
1:E:203:ALA:O	1:E:207:ILE:HG13	2.18	0.44
1:D:357:ILE:CG2	1:D:358:GLU:N	2.80	0.44
1:F:149:VAL:O	1:F:153:LYS:HG2	2.17	0.44
1:D:179:VAL:HG13	1:D:187:VAL:HG21	1.99	0.44
1:F:360:ASP:HB3	1:F:363:LEU:HD12	2.00	0.44
1:G:14:PRO:HB3	1:G:20:VAL:HG22	2.00	0.44
1:H:6:LEU:O	1:H:57:LYS:HE3	2.17	0.44
1:C:6:LEU:O	1:C:57:LYS:HE3	2.18	0.44
1:C:266:ASN:C	1:C:266:ASN:ND2	2.69	0.44
1:A:158:PHE:CZ	1:A:327:GLU:HG3	2.53	0.44
1:D:154:LEU:HA	1:D:158:PHE:O	2.18	0.44
1:D:125:LYS:HD2	1:D:128:ILE:HG22	1.99	0.44
1:C:145:SER:HB3	4:C:410:HOH:O	2.17	0.44
1:B:113:ASP:OD1	1:B:353:LYS:HE2	2.17	0.44
1:B:360:ASP:HB3	1:B:363:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:ILE:O	1:H:272:ILE:HG13	2.18	0.44
1:H:125:LYS:HD2	1:H:128:ILE:HG22	1.99	0.44
1:H:149:VAL:O	1:H:153:LYS:HG2	2.18	0.44
1:E:158:PHE:CZ	1:E:327:GLU:HG3	2.52	0.44
1:H:179:VAL:HG13	1:H:187:VAL:HG21	1.98	0.44
1:F:125:LYS:HD2	1:F:128:ILE:HG22	1.98	0.44
1:G:113:ASP:OD1	1:G:353:LYS:HE2	2.17	0.44
1:B:203:ALA:O	1:B:207:ILE:HG13	2.17	0.44
1:C:123:ARG:NH1	1:C:126:GLU:OE2	2.51	0.43
1:F:113:ASP:OD1	1:F:353:LYS:HE2	2.18	0.43
1:A:113:ASP:OD1	1:A:353:LYS:HE2	2.17	0.43
1:H:21:ASN:ND2	1:H:329:TYR:HE1	2.15	0.43
1:F:158:PHE:CZ	1:F:327:GLU:HG3	2.52	0.43
1:G:123:ARG:NH1	1:G:126:GLU:OE2	2.51	0.43
1:F:6:LEU:O	1:F:57:LYS:HE3	2.19	0.43
1:E:14:PRO:HB3	1:E:20:VAL:HG22	2.00	0.43
1:D:167:LYS:HZ3	1:D:380:HIS:CD2	2.36	0.43
1:A:16:HIS:HE1	4:A:412:HOH:O	2.02	0.43
1:B:272:ILE:HG13	1:B:272:ILE:O	2.18	0.43
1:C:113:ASP:OD1	1:C:353:LYS:HE2	2.18	0.43
1:D:22:LYS:CE	1:D:369:VAL:HG11	2.46	0.43
1:B:68:ASN:ND2	1:B:70:PHE:H	2.16	0.43
1:C:149:VAL:O	1:C:153:LYS:HG2	2.17	0.43
1:G:6:LEU:O	1:G:57:LYS:HE3	2.18	0.43
1:F:266:ASN:C	1:F:266:ASN:ND2	2.68	0.43
1:A:341:LYS:HB3	1:A:346:TYR:HE2	1.84	0.43
1:E:6:LEU:O	1:E:57:LYS:HE3	2.19	0.43
1:B:14:PRO:HB3	1:B:20:VAL:HG22	2.00	0.43
1:H:14:PRO:HB3	1:H:20:VAL:HG22	2.01	0.43
1:B:6:LEU:O	1:B:57:LYS:HE3	2.17	0.43
1:F:341:LYS:HB3	1:F:346:TYR:HE2	1.84	0.43
1:C:167:LYS:HZ3	1:C:380:HIS:CD2	2.36	0.43
1:H:158:PHE:CZ	1:H:327:GLU:HG3	2.53	0.43
1:E:149:VAL:O	1:E:153:LYS:HG2	2.18	0.43
1:A:167:LYS:HZ1	1:A:380:HIS:HD2	1.67	0.43
1:A:68:ASN:ND2	1:A:68:ASN:C	2.72	0.43
1:G:203:ALA:O	1:G:207:ILE:HG13	2.18	0.43
1:G:167:LYS:HZ3	1:G:380:HIS:CD2	2.37	0.43
1:C:357:ILE:HA	1:C:357:ILE:HD13	1.90	0.43
1:B:266:ASN:ND2	1:B:266:ASN:C	2.69	0.43
1:D:68:ASN:ND2	1:D:70:PHE:H	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ILE:HA	1:B:357:ILE:HD13	1.90	0.42
1:C:203:ALA:O	1:C:207:ILE:HG13	2.19	0.42
1:C:68:ASN:ND2	1:C:70:PHE:H	2.17	0.42
1:G:158:PHE:CZ	1:G:327:GLU:HG3	2.54	0.42
1:B:205:ARG:HD3	1:H:240:ASP:O	2.19	0.42
1:A:6:LEU:O	1:A:57:LYS:HE3	2.19	0.42
1:G:272:ILE:HG13	1:G:272:ILE:O	2.19	0.42
1:H:123:ARG:NH1	1:H:126:GLU:OE2	2.51	0.42
1:B:149:VAL:O	1:B:153:LYS:HG2	2.19	0.42
1:E:371:ASP:HB2	4:E:429:HOH:O	2.20	0.42
1:E:123:ARG:NH1	1:E:126:GLU:OE2	2.51	0.42
1:F:123:ARG:NH1	1:F:126:GLU:OE2	2.52	0.42
1:B:123:ARG:NH1	1:B:126:GLU:OE2	2.51	0.42
1:E:22:LYS:CE	1:E:369:VAL:HG11	2.47	0.42
1:A:59:GLY:O	1:A:62:SER:HB3	2.19	0.42
1:F:117:SER:OG	1:F:309:HIS:CD2	2.66	0.42
1:C:21:ASN:ND2	1:C:329:TYR:HE1	2.16	0.42
1:F:151:ARG:NH1	1:F:182:GLU:OE2	2.41	0.42
1:A:123:ARG:NH1	1:A:126:GLU:OE2	2.51	0.42
1:C:167:LYS:HZ3	1:C:380:HIS:HD2	1.66	0.42
1:H:154:LEU:HA	1:H:158:PHE:O	2.20	0.42
1:D:203:ALA:O	1:D:207:ILE:HG13	2.19	0.42
1:C:14:PRO:HB3	1:C:20:VAL:HG22	2.00	0.42
1:H:203:ALA:O	1:H:207:ILE:HG13	2.20	0.42
1:C:154:LEU:HA	1:C:158:PHE:O	2.20	0.42
1:A:369:VAL:CG1	1:A:370:PRO:HD2	2.50	0.42
1:E:297:THR:HA	2:E:392:LMR:O2	2.20	0.42
1:D:341:LYS:HB3	1:D:346:TYR:HE2	1.85	0.42
1:G:326:PRO:HG2	1:G:338:VAL:HG22	2.02	0.42
1:H:167:LYS:HZ3	1:H:380:HIS:CD2	2.36	0.42
1:B:22:LYS:CE	1:B:369:VAL:HG11	2.47	0.42
1:G:21:ASN:ND2	1:G:329:TYR:HE1	2.18	0.42
1:G:357:ILE:HA	1:G:357:ILE:HD13	1.88	0.42
1:C:272:ILE:HG13	1:C:272:ILE:O	2.19	0.42
1:H:299:GLU:OE2	1:H:307:MET:SD	2.78	0.42
1:D:158:PHE:CZ	1:D:327:GLU:HG3	2.53	0.41
1:B:154:LEU:HA	1:B:158:PHE:O	2.19	0.41
1:C:102:ASN:HD22	1:C:102:ASN:C	2.13	0.41
1:G:167:LYS:HZ1	1:G:380:HIS:HD2	1.63	0.41
1:F:154:LEU:HA	1:F:158:PHE:O	2.20	0.41
1:E:369:VAL:CG1	1:E:370:PRO:HD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:GLY:O	1:H:62:SER:HB3	2.20	0.41
1:A:312:CYS:SG	1:A:347:ALA:HB2	2.60	0.41
1:F:203:ALA:O	1:F:207:ILE:HG13	2.20	0.41
1:D:14:PRO:HB3	1:D:20:VAL:HG22	2.02	0.41
1:F:21:ASN:ND2	1:F:329:TYR:HE1	2.19	0.41
1:D:21:ASN:ND2	1:D:329:TYR:HE1	2.18	0.41
1:G:86:THR:O	1:G:87:MET:CB	2.69	0.41
1:H:86:THR:O	1:H:87:MET:CB	2.67	0.41
1:G:341:LYS:HB3	1:G:346:TYR:HE2	1.86	0.41
1:A:203:ALA:O	1:A:207:ILE:HG13	2.20	0.41
1:E:151:ARG:NH1	1:E:182:GLU:OE2	2.44	0.41
1:G:266:ASN:ND2	1:G:266:ASN:C	2.70	0.41
1:C:226:ARG:HG2	1:C:248:TRP:CH2	2.56	0.41
1:H:167:LYS:HZ3	1:H:380:HIS:HD2	1.65	0.41
1:A:21:ASN:ND2	1:A:329:TYR:HE1	2.19	0.41
1:A:86:THR:O	1:A:87:MET:CB	2.68	0.41
1:C:322:ASP:N	1:C:323:PRO:CD	2.83	0.41
1:D:59:GLY:O	1:D:62:SER:HB3	2.20	0.41
1:F:48:LEU:HD22	1:H:82:ASN:ND2	2.36	0.41
1:E:38:GLY:HA3	1:E:103:ALA:HB2	2.03	0.41
1:D:117:SER:OG	1:D:309:HIS:CD2	2.65	0.41
1:E:322:ASP:N	1:E:323:PRO:CD	2.84	0.41
1:C:297:THR:HA	2:C:392:LMR:O2	2.20	0.41
1:F:59:GLY:O	1:F:62:SER:HB3	2.21	0.41
1:D:326:PRO:HG2	1:D:338:VAL:HG22	2.03	0.41
1:C:86:THR:O	1:C:87:MET:CB	2.68	0.41
1:A:154:LEU:HA	1:A:158:PHE:O	2.20	0.41
1:E:154:LEU:HA	1:E:158:PHE:O	2.20	0.41
1:A:82:ASN:HD22	1:C:48:LEU:HD22	1.86	0.41
1:E:59:GLY:O	1:E:62:SER:HB3	2.21	0.41
1:A:241:TYR:HA	1:A:242:PRO:HD3	1.93	0.41
1:B:312:CYS:SG	1:B:347:ALA:HB2	2.61	0.41
1:C:22:LYS:CE	1:C:369:VAL:HG11	2.48	0.41
1:H:22:LYS:CE	1:H:369:VAL:HG11	2.48	0.41
1:D:322:ASP:N	1:D:323:PRO:HD2	2.35	0.41
1:C:147:LEU:HD11	1:C:178:ARG:HB3	2.03	0.41
1:F:272:ILE:HG13	1:F:272:ILE:O	2.21	0.41
1:F:14:PRO:HB3	1:F:20:VAL:HG22	2.02	0.41
1:E:86:THR:O	1:E:87:MET:CB	2.68	0.40
1:B:322:ASP:N	1:B:323:PRO:CD	2.85	0.40
1:E:341:LYS:HB3	1:E:346:TYR:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASN:ND2	1:G:48:LEU:HD22	2.37	0.40
1:D:38:GLY:HA3	1:D:103:ALA:HB2	2.03	0.40
1:H:38:GLY:HA3	1:H:103:ALA:HB2	2.03	0.40
1:E:68:ASN:C	1:E:68:ASN:ND2	2.75	0.40
1:G:154:LEU:HA	1:G:158:PHE:O	2.21	0.40
1:D:6:LEU:O	1:D:57:LYS:HE3	2.20	0.40
1:H:68:ASN:C	1:H:68:ASN:ND2	2.74	0.40
1:F:322:ASP:N	1:F:323:PRO:CD	2.85	0.40
1:A:266:ASN:ND2	1:A:266:ASN:C	2.68	0.40
1:C:240:ASP:O	1:E:205:ARG:HD3	2.22	0.40
1:H:304:THR:HA	1:H:307:MET:HG2	2.04	0.40
1:H:226:ARG:HG2	1:H:248:TRP:CH2	2.57	0.40
1:B:341:LYS:HB3	1:B:346:TYR:HE2	1.87	0.40
1:A:48:LEU:HD22	1:C:82:ASN:ND2	2.37	0.40
1:G:322:ASP:N	1:G:323:PRO:HD2	2.37	0.40
1:C:322:ASP:N	1:C:323:PRO:HD2	2.36	0.40
1:D:322:ASP:N	1:D:323:PRO:CD	2.84	0.40
1:D:312:CYS:SG	1:D:347:ALA:HB2	2.62	0.40
1:D:48:LEU:HD22	1:E:82:ASN:ND2	2.36	0.40
1:H:382:LEU:HA	1:H:382:LEU:HD23	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/391 (98%)	374 (97%)	9 (2%)	2 (0%)	34	35
1	B	385/391 (98%)	374 (97%)	9 (2%)	2 (0%)	34	35
1	C	385/391 (98%)	373 (97%)	10 (3%)	2 (0%)	34	35
1	D	385/391 (98%)	373 (97%)	10 (3%)	2 (0%)	34	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	385/391 (98%)	372 (97%)	11 (3%)	2 (0%)	34	35
1	F	385/391 (98%)	373 (97%)	11 (3%)	1 (0%)	46	50
1	G	385/391 (98%)	373 (97%)	10 (3%)	2 (0%)	34	35
1	H	385/391 (98%)	371 (96%)	13 (3%)	1 (0%)	46	50
All	All	3080/3128 (98%)	2983 (97%)	83 (3%)	14 (0%)	34	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	B	42	ASP
1	C	42	ASP
1	D	42	ASP
1	E	42	ASP
1	F	42	ASP
1	G	42	ASP
1	H	42	ASP
1	A	322	ASP
1	B	322	ASP
1	C	322	ASP
1	D	322	ASP
1	E	322	ASP
1	G	322	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/345 (99%)	328 (96%)	13 (4%)	40	49
1	B	341/345 (99%)	328 (96%)	13 (4%)	40	49
1	C	341/345 (99%)	328 (96%)	13 (4%)	40	49
1	D	341/345 (99%)	328 (96%)	13 (4%)	40	49
1	E	341/345 (99%)	328 (96%)	13 (4%)	40	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	341/345 (99%)	328 (96%)	13 (4%)	40	49
1	G	341/345 (99%)	328 (96%)	13 (4%)	40	49
1	H	341/345 (99%)	328 (96%)	13 (4%)	40	49
All	All	2728/2760 (99%)	2624 (96%)	104 (4%)	40	49

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	68	ASN
1	A	87	MET
1	A	102	ASN
1	A	107	LEU
1	A	141	GLU
1	A	190	LYS
1	A	237	LEU
1	A	239	THR
1	A	259	LYS
1	A	266	ASN
1	A	355	LEU
1	A	368	GLN
1	B	1	MET
1	B	68	ASN
1	B	87	MET
1	B	102	ASN
1	B	107	LEU
1	B	141	GLU
1	B	190	LYS
1	B	237	LEU
1	B	239	THR
1	B	259	LYS
1	B	266	ASN
1	B	355	LEU
1	B	368	GLN
1	C	1	MET
1	C	68	ASN
1	C	87	MET
1	C	102	ASN
1	C	107	LEU
1	C	141	GLU
1	C	190	LYS

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Mol	Chain	Res	Type
1	C	237	LEU
1	C	239	THR
1	C	259	LYS
1	C	266	ASN
1	C	355	LEU
1	C	368	GLN
1	D	1	MET
1	D	68	ASN
1	D	87	MET
1	D	102	ASN
1	D	107	LEU
1	D	141	GLU
1	D	190	LYS
1	D	237	LEU
1	D	239	THR
1	D	259	LYS
1	D	266	ASN
1	D	355	LEU
1	D	368	GLN
1	E	1	MET
1	E	68	ASN
1	E	87	MET
1	E	102	ASN
1	E	107	LEU
1	E	141	GLU
1	E	190	LYS
1	E	237	LEU
1	E	239	THR
1	E	259	LYS
1	E	266	ASN
1	E	355	LEU
1	E	368	GLN
1	F	1	MET
1	F	68	ASN
1	F	87	MET
1	F	102	ASN
1	F	107	LEU
1	F	141	GLU
1	F	190	LYS
1	F	237	LEU
1	F	239	THR
1	F	259	LYS

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Mol	Chain	Res	Type
1	F	266	ASN
1	F	355	LEU
1	F	368	GLN
1	G	1	MET
1	G	68	ASN
1	G	87	MET
1	G	102	ASN
1	G	107	LEU
1	G	141	GLU
1	G	190	LYS
1	G	237	LEU
1	G	239	THR
1	G	259	LYS
1	G	266	ASN
1	G	355	LEU
1	G	368	GLN
1	H	1	MET
1	H	68	ASN
1	H	87	MET
1	H	102	ASN
1	H	107	LEU
1	H	141	GLU
1	H	190	LYS
1	H	237	LEU
1	H	239	THR
1	H	259	LYS
1	H	266	ASN
1	H	355	LEU
1	H	368	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	21	ASN
1	A	68	ASN
1	A	82	ASN
1	A	102	ASN
1	A	146	ASN
1	A	152	GLN
1	A	196	HIS
1	A	199	ASN

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Mol	Chain	Res	Type
1	A	254	GLN
1	A	266	ASN
1	A	309	HIS
1	A	368	GLN
1	A	376	ASN
1	A	380	HIS
1	B	16	HIS
1	B	21	ASN
1	B	68	ASN
1	B	82	ASN
1	B	102	ASN
1	B	146	ASN
1	B	152	GLN
1	B	196	HIS
1	B	199	ASN
1	B	254	GLN
1	B	266	ASN
1	B	309	HIS
1	B	368	GLN
1	B	376	ASN
1	B	380	HIS
1	C	16	HIS
1	C	21	ASN
1	C	68	ASN
1	C	102	ASN
1	C	146	ASN
1	C	152	GLN
1	C	196	HIS
1	C	199	ASN
1	C	254	GLN
1	C	266	ASN
1	C	309	HIS
1	C	368	GLN
1	C	376	ASN
1	C	380	HIS
1	D	16	HIS
1	D	21	ASN
1	D	68	ASN
1	D	102	ASN
1	D	146	ASN
1	D	152	GLN
1	D	196	HIS

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Mol	Chain	Res	Type
1	D	199	ASN
1	D	254	GLN
1	D	266	ASN
1	D	309	HIS
1	D	368	GLN
1	D	376	ASN
1	D	380	HIS
1	E	16	HIS
1	E	21	ASN
1	E	68	ASN
1	E	82	ASN
1	E	102	ASN
1	E	146	ASN
1	E	152	GLN
1	E	196	HIS
1	E	199	ASN
1	E	254	GLN
1	E	266	ASN
1	E	309	HIS
1	E	368	GLN
1	E	376	ASN
1	E	380	HIS
1	F	16	HIS
1	F	21	ASN
1	F	68	ASN
1	F	82	ASN
1	F	102	ASN
1	F	146	ASN
1	F	152	GLN
1	F	196	HIS
1	F	199	ASN
1	F	254	GLN
1	F	266	ASN
1	F	309	HIS
1	F	368	GLN
1	F	376	ASN
1	F	380	HIS
1	G	16	HIS
1	G	21	ASN
1	G	68	ASN
1	G	82	ASN
1	G	102	ASN

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Mol	Chain	Res	Type
1	G	146	ASN
1	G	152	GLN
1	G	196	HIS
1	G	199	ASN
1	G	254	GLN
1	G	266	ASN
1	G	309	HIS
1	G	368	GLN
1	G	376	ASN
1	G	380	HIS
1	H	16	HIS
1	H	21	ASN
1	H	68	ASN
1	H	82	ASN
1	H	102	ASN
1	H	146	ASN
1	H	152	GLN
1	H	196	HIS
1	H	199	ASN
1	H	254	GLN
1	H	266	ASN
1	H	309	HIS
1	H	368	GLN
1	H	376	ASN
1	H	380	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LMR	A	392	3	1,8,8	1.45	0	2,10,10	0.86	0
2	LMR	B	392	3	1,8,8	1.58	0	2,10,10	0.96	0
2	LMR	C	392	3	1,8,8	1.49	0	2,10,10	0.74	0
2	LMR	D	392	3	1,8,8	1.33	0	2,10,10	1.36	0
2	LMR	E	392	3	1,8,8	1.32	0	2,10,10	0.80	0
2	LMR	F	392	3	1,8,8	1.70	0	2,10,10	0.94	0
2	LMR	G	392	3	1,8,8	1.45	0	2,10,10	0.77	0
2	LMR	H	392	3	1,8,8	1.42	0	2,10,10	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMR	A	392	3	-	0/2/8/8	0/0/0/0
2	LMR	B	392	3	-	0/2/8/8	0/0/0/0
2	LMR	C	392	3	-	0/2/8/8	0/0/0/0
2	LMR	D	392	3	-	0/2/8/8	0/0/0/0
2	LMR	E	392	3	-	0/2/8/8	0/0/0/0
2	LMR	F	392	3	-	0/2/8/8	0/0/0/0
2	LMR	G	392	3	-	0/2/8/8	0/0/0/0
2	LMR	H	392	3	-	0/2/8/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	392	LMR	1	0
2	C	392	LMR	1	0
2	E	392	LMR	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	387/391 (98%)	-0.21	1 (0%) 94 94	28, 42, 54, 67	0
1	B	387/391 (98%)	-0.24	0 100 100	30, 43, 57, 71	0
1	C	387/391 (98%)	-0.19	0 100 100	31, 44, 59, 71	0
1	D	387/391 (98%)	-0.20	0 100 100	30, 42, 54, 62	0
1	E	387/391 (98%)	-0.18	0 100 100	29, 43, 57, 70	0
1	F	387/391 (98%)	-0.20	0 100 100	28, 41, 53, 64	0
1	G	387/391 (98%)	-0.21	0 100 100	30, 42, 54, 67	0
1	H	387/391 (98%)	-0.16	1 (0%) 94 94	31, 44, 58, 68	0
All	All	3096/3128 (98%)	-0.20	2 (0%) 95 95	28, 43, 57, 71	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	376	ASN	2.4
1	A	1	MET	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	F	393	1/1	0.98	0.17	7.61	18,18,18,18	0
3	MG	H	393	1/1	0.98	0.15	3.82	25,25,25,25	0
2	LMR	G	392	9/9	0.88	0.15	2.74	41,45,47,47	0
3	MG	E	393	1/1	0.95	0.14	1.63	20,20,20,20	0
2	LMR	D	392	9/9	0.90	0.12	1.61	42,43,44,45	0
2	LMR	C	392	9/9	0.88	0.14	1.31	51,54,56,57	0
3	MG	G	393	1/1	0.98	0.12	1.26	22,22,22,22	0
3	MG	A	393	1/1	0.96	0.12	1.06	19,19,19,19	0
2	LMR	E	392	9/9	0.89	0.13	1.02	47,50,52,53	0
2	LMR	F	392	9/9	0.91	0.13	0.79	40,42,45,46	0
2	LMR	B	392	9/9	0.89	0.11	-0.08	44,46,52,53	0
3	MG	C	393	1/1	0.95	0.10	-0.26	24,24,24,24	0
2	LMR	A	392	9/9	0.93	0.11	-0.37	34,38,39,41	0
2	LMR	H	392	9/9	0.91	0.11	-0.44	55,56,57,57	0
3	MG	B	393	1/1	0.96	0.09	-1.05	20,20,20,20	0
3	MG	D	393	1/1	0.98	0.10	-1.55	18,18,18,18	0

## 6.5 Other polymers

There are no such residues in this entry.